

10/535,136

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal201txs

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 JAN 08 CHEMLIST enhanced with New Zealand Inventory of Chemicals  
NEWS 3 JAN 16 CA/CAPLUS Company Name Thesaurus enhanced and reloaded  
NEWS 4 JAN 16 IPC version 2007.01 thesaurus available on STN  
NEWS 5 JAN 16 WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification  
data  
NEWS 6 JAN 22 CA/CAPLUS updated with revised CAS roles  
NEWS 7 JAN 22 CA/CAPLUS enhanced with patent applications from India  
NEWS 8 JAN 29 PHAR reloaded with new search and display fields  
NEWS 9 JAN 29 CAS Registry Number crossover limit increased to 300,000  
in  
multiple databases  
NEWS 10 FEB 15 PATDPASPC enhanced with Drug Approval numbers  
NEWS 11 FEB 15 RUSSIAPAT enhanced with pre-1994 records  
NEWS 12 FEB 23 KOREAPAT enhanced with IPC 8 features and functionality  
NEWS 13 FEB 26 MEDLINE reloaded with enhancements  
NEWS 14 FEB 26 EMBASE enhanced with Clinical Trial Number field  
NEWS 15 FEB 26 TOXCENTER enhanced with reloaded MEDLINE  
NEWS 16 FEB 26 IFICDB/IFIPAT/IFIUDB reloaded with enhancements  
NEWS 17 FEB 26 CAS Registry Number crossover limit increased from 10,000  
to 300,000 in multiple databases  
NEWS 18 MAR 15 WPIDS/WPIX enhanced with new FRAGHITSTR display format  
NEWS 19 MAR 16 CASREACT coverage extended  
NEWS 20 MAR 20 MARPAT now updated daily  
NEWS 21 MAR 22 LWPI reloaded  
NEWS 22 MAR 30 RDISCLOSURE reloaded with enhancements  
NEWS 23 APR 02 JICST-EPLUS removed from database clusters and STN  
NEWS 24 APR 30 GENBANK reloaded and enhanced with Genome Project ID field  
NEWS 25 APR 30 CHEMCATS enhanced with 1.2 million new records  
NEWS 26 APR 30 CA/CAPLUS enhanced with 1870-1889 U.S. patent records  
NEWS 27 APR 30 INPADOC replaced by INPADOCDB on STN  
NEWS 28 MAY 01 New CAS web site launched  
  
NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT  
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

10/535,136

NEWS HOURS      STN Operating Hours Plus Help Desk Availability  
NEWS LOGIN      Welcome Banner and News Items  
NEWS IPC8        For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 14:10:02 ON 02 MAY 2007

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:10:21 ON 02 MAY 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8

DICTIONARY FILE UPDATES: 1 MAY 2007 HIGHEST RN 934050-43-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

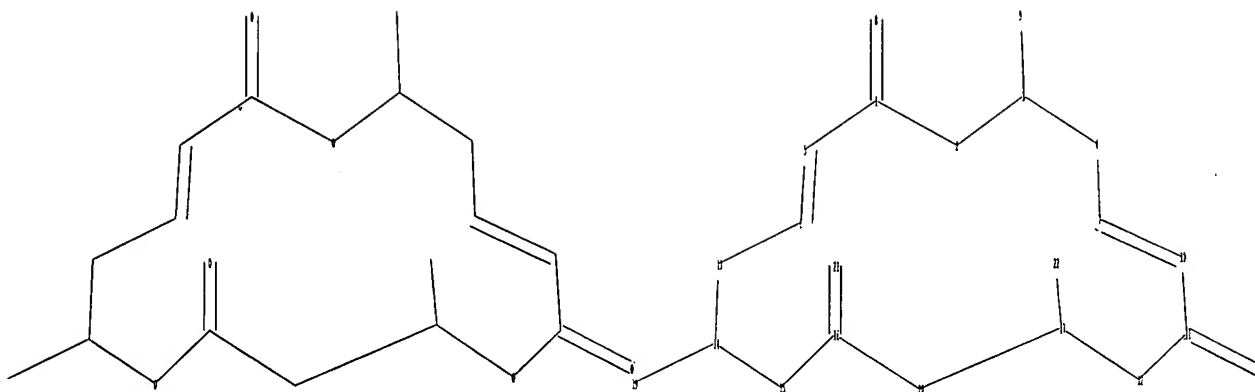
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10535136.str

10/535,136



chain nodes :  
8 9 18 19 21 22  
ring nodes :  
1 2 3 4 5 6 7 10 11 12 13 14 15 16 17 20  
chain bonds :  
1-8 3-9 11-18 14-19 16-21 17-22  
ring bonds :  
1-2 1-5 2-3 3-4 4-7 5-6 6-13 7-10 10-11 11-12 12-17 13-14 14-15  
15-16 16-20 17-20  
exact/norm bonds :  
1-8 11-18 16-21  
exact bonds :  
1-2 1-5 2-3 3-4 3-9 4-7 5-6 6-13 7-10 10-11 11-12 12-17 13-14  
14-15 14-19 15-16 16-20 17-20 17-22  
isolated ring systems :  
containing 1 :

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:CLASS 9:CLASS  
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom  
18:CLASS 19:CLASS 20:Atom 21:CLASS 22:CLASS

L1 STRUCTURE UPLOADED

10/535,136

=> s l1

SAMPLE SEARCH INITIATED 14:10:40 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 414 TO ITERATE

100.0% PROCESSED 414 ITERATIONS 3 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 7060 TO 9500  
PROJECTED ANSWERS: 3 TO 163

L2 3 SEA SSS SAM L1

=> s l1 ful

FULL SEARCH INITIATED 14:10:48 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 8737 TO ITERATE

100.0% PROCESSED 8737 ITERATIONS 120 ANSWERS  
SEARCH TIME: 00.00.01

L3 120 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.10	172.31

FILE 'CAPLUS' ENTERED AT 14:10:59 ON 02 MAY 2007  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 2 May 2007 VOL 146 ISS 19  
FILE LAST UPDATED: 1 May 2007 (20070501/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

10/535,136

=> s 13

L4 46 L3

=> s 14 and (process? or method or make or syntheses? or prepar? or making)

4068973 PROCESS?

3384211 METHOD

1365704 METHODS

4365201 METHOD

(METHOD OR METHODS)

259526 MAKE

199903 MAKES

445217 MAKE

(MAKE OR MAKES)

1619265 SYNTHES?

1761757 PREPAR?

129831 PREP

2255 PREPS

131873 PREP

(PREP OR PREPS)

2081783 PREPD

5 PREPDS

2081787 PREPD

(PREPD OR PREPDS)

137822 PREPG

12 PREPGS

137833 PREPG

(PREPG OR PREPGS)

2803951 PREPN

208693 PREPNS

2961214 PREPN

(PREPN OR PREPNS)

4952014 PREPAR?

(PREPAR? OR PREP OR PREPD OR PREPG OR PREPN)

310976 MAKING

33 MAKINGS

311003 MAKING

(MAKING OR MAKINGS)

L5 38 L4 AND (PROCESS? OR METHOD OR MAKE OR SYNTHES? OR PREPAR? OR MAKING)

=> s 15 and 3-hydroxybutyrate

6885735 3

14029 HYDROXYBUTYRATE

165 HYDROXYBUTYRATES

14092 HYDROXYBUTYRATE

(HYDROXYBUTYRATE OR HYDROXYBUTYRATES)

4710 3-HYDROXYBUTYRATE

(3(W)HYDROXYBUTYRATE)

L6 4 L5 AND 3-HYDROXYBUTYRATE

=> d 15 ibib hitstr abs 1-38

L5 ANSWER 10 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2004:467880 CAPLUS  
 DOCUMENT NUMBER: 141:38807  
 TITLE: A process for the preparation of  
 macrosphelide scaffold via macrolactonization  
 INVENTOR(S): Nemoto, Hideo; Matsuya, Yuji  
 PATENT ASSIGNEE(S): Lead Chemical Co., Ltd., Japan  
 SOURCE: PCT Int. Appl., 31 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

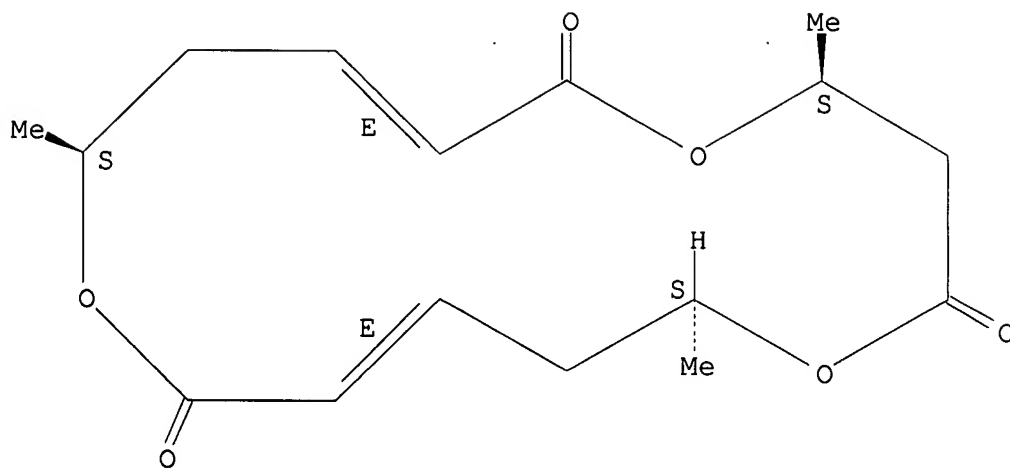
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004048360	A1	20040610	WO 2002-JP12304	20021126
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2002355031	A1	20040618	AU 2002-355031	20021126
US 2006030720	A1	20060209	US 2005-535136	20050622
PRIORITY APPLN. INFO.:			WO 2002-JP12304	A 20021126

IT 554420-08-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (process for the preparation of macrosphelide scaffold  
 via macrolactonization)

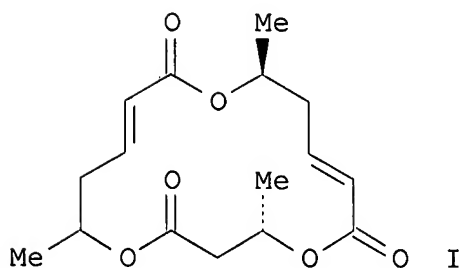
RN 554420-08-5 CAPLUS

CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12-trione,  
 4,10,16-trimethyl-,  
 (4S,7E,10S,13E,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).  
 Double bond geometry as shown.



GI



AB A process for the preparation of macrocyclic scaffold I via macrolactonization was provided. For example, to a mixture of (+)-1-tert-butoxycarbonylpent-1-en-4-yl 5-hydroxyhex-2-enoate (50 mg), 3-tert-butyltrimethylsilyloxybutanoic acid (43 mg) and DMAP (2 mg) in CH<sub>2</sub>Cl<sub>2</sub> (2 mL) was added DCC (55 mg) at 0 °C, and stirred at room temperature for 3 h. Aqueous work-up afforded (-)-1-tert-butoxycarbonylpent-1-en-4-yl 5-[3-(tert-butyltrimethylsilyloxy)butyloxy]hex-2-enoate (II) (81 mg). Desilylation and hydrolysis of compound II (500 mg) using thioanisole (12.5 mL) and trifluoroacetic acid (2.5 mL) in CH<sub>2</sub>Cl<sub>2</sub> at room temperature for 1 h gave (-)-5-[5-(3-hydroxybutyloxy)hex-2-enoyloxy]hex-2-enoic acid (III) (273 mg). A mixture of compound III (40 mg), triethylamine (73 mg) and 2,4,6-trichlorobenzoyl chloride (146 mg) in toluene (10 mL) was stirred at room temperature for 1 h, then DMAP (170 mg) was added slowly over a period of 2

10/535,136

h at 80 °C. After basic work-up, purification on silica-gel furnished  
macrospinelide scaffold I (34 mg).

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR  
THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

L5 ANSWER 22 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:862446 CAPLUS

DOCUMENT NUMBER: 138:271895

TITLE: The total synthesis of macrospinelides A and  
E from carbohydrate precursors

AUTHOR(S): Sharma, G. V. M.; Mouli, Ch. Chandra

CORPORATE SOURCE: Organic Chemistry Division-III, Discovery  
Laboratory,

D-211, Indian Institute of Chemical Technology,  
Hyderabad, 500 007, India

SOURCE: Tetrahedron Letters (2002), 43(50), 9159-9161  
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:271895

IT 503026-46-8P 503026-52-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
RACT

(Reactant or reagent)

(total synthesis of macrospinelides A and E from carbohydrate  
precursors)

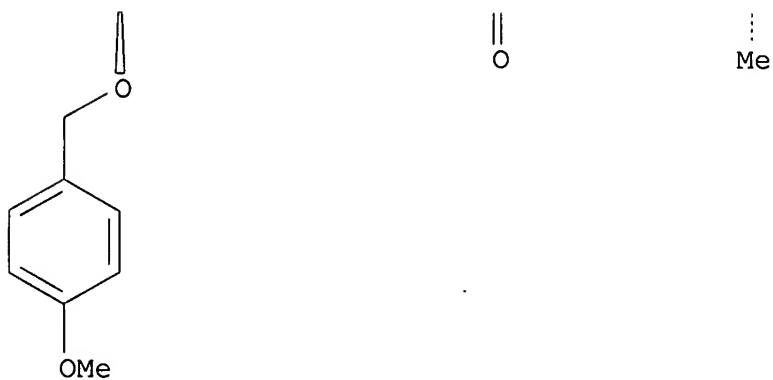
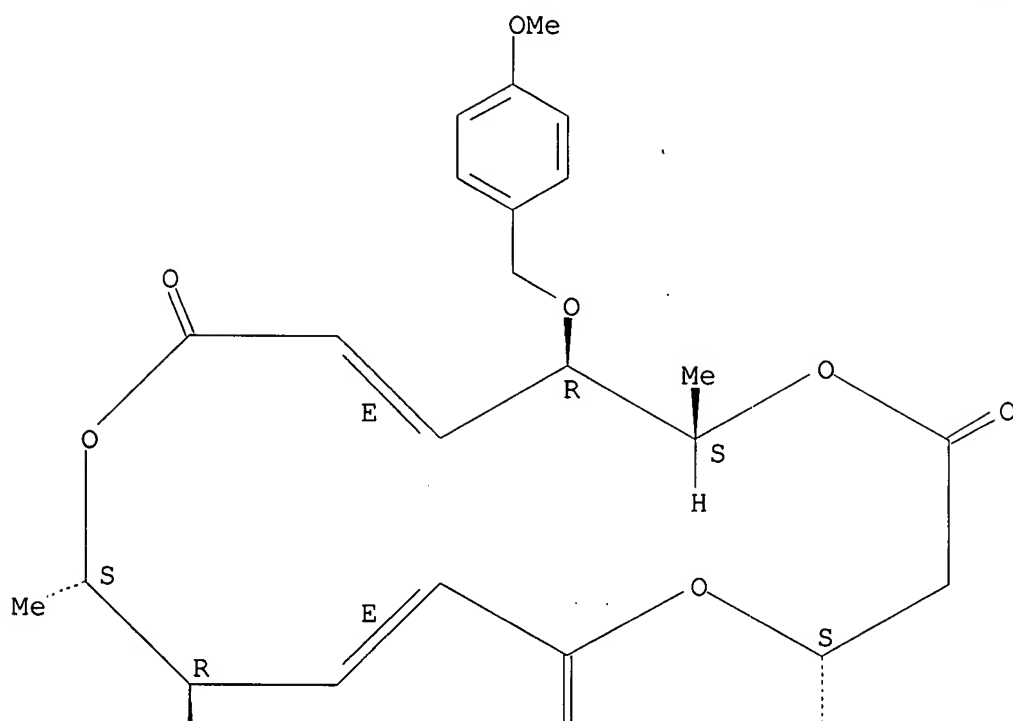
RN 503026-46-8 CAPLUS

CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12-trione, 9,15-bis[(4-  
methoxyphenyl)methoxy]-4,10,16-trimethyl-, (4S,7E,9R,10S,13E,15R,16S)-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

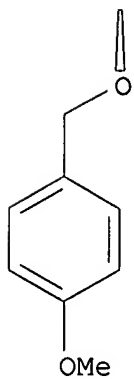
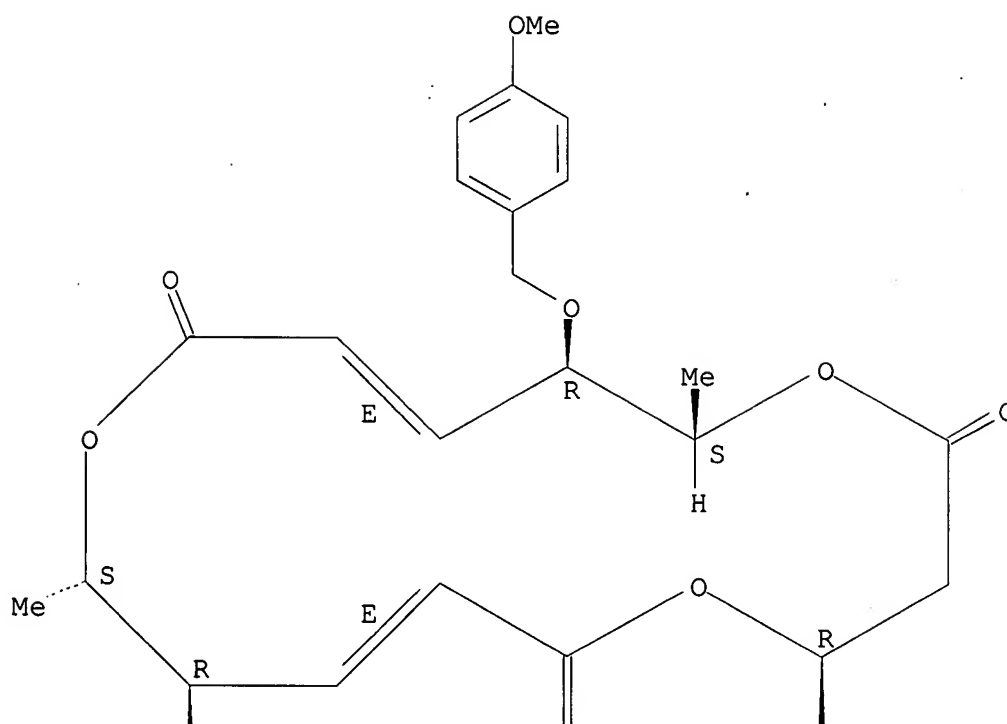
Double bond geometry as shown.





RN 503026-52-6 CAPLUS  
 CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12-trione, 9,15-bis[(4-methoxyphenyl)methoxy]-4,10,16-trimethyl-, (4R,7E,9R,10S,13E,15R,16S)-(9CI) (CA INDEX NAME)

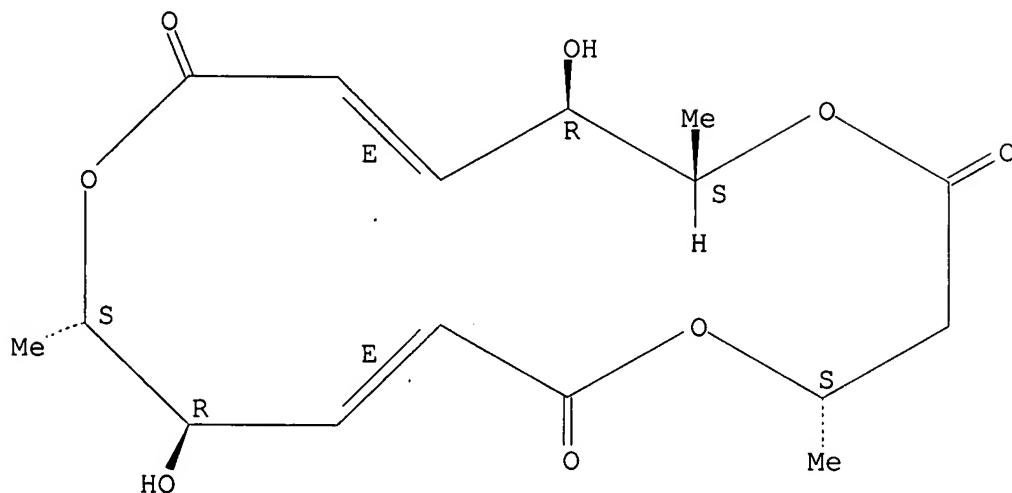
Absolute stereochemistry.  
 Double bond geometry as shown.



IT 172923-77-2P 200335-76-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (total synthesis of macrospinelides A and E from carbohydrate  
 precursors)  
 RN 172923-77-2 CAPLUS  
 CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12-trione, 9,15-dihydroxy-  
 4,10,16-trimethyl-, (4S,7E,9R,10S,13E,15R,16S)- (CA INDEX NAME)

10/535,136

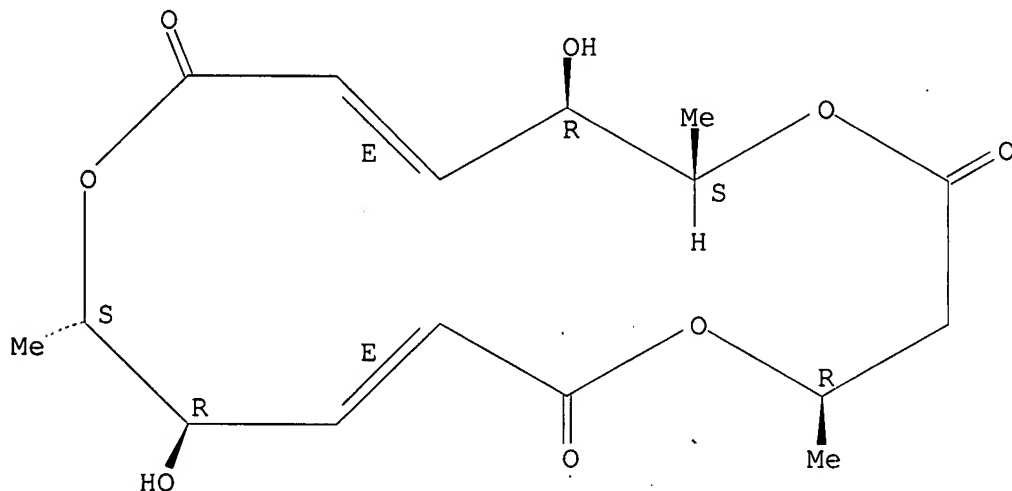
Absolute stereochemistry. Rotation (+).  
Double bond geometry as shown.



RN 200335-76-8 CAPLUS

CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12-trione, 9,15-dihydroxy-4,10,16-trimethyl-, (4R,7E,9R,10S,13E,15R,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).  
Double bond geometry as shown.



AB The total synthesis of macrolide antibiotics, macrosphelide A and E has been achieved starting from L-(+)-arabinose and (3S)- or (3R)-3-hydroxybutyric acid via Yamaguchi macrolactonization of intermediates.

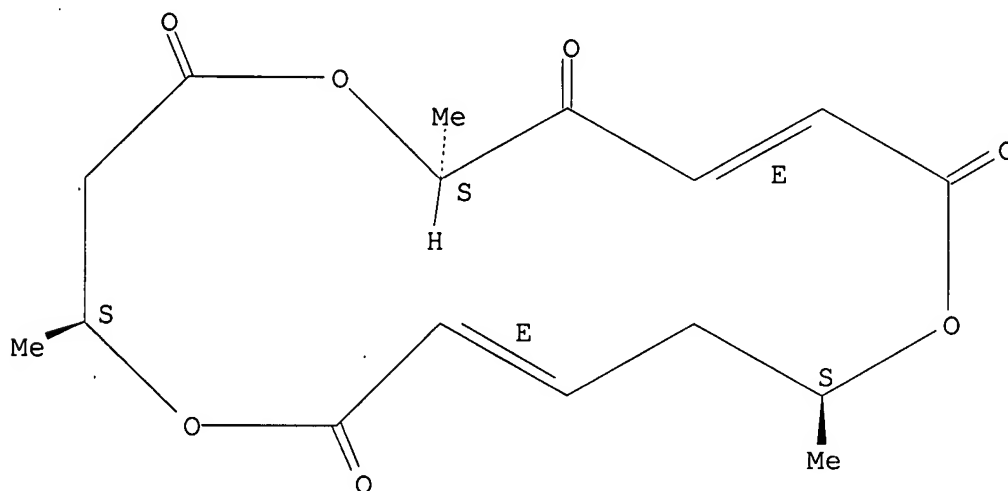
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L5 ANSWER 30 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2001:246247 CAPLUS  
DOCUMENT NUMBER: 135:46021  
TITLE: First total synthesis of macrosphelides C  
and F  
AUTHOR(S): Kobayashi, Y.; Acharya, H. P.  
CORPORATE SOURCE: Department of Biomolecular Engineering, 4259  
Nagatsuta-cho, Tokyo Institute of Technology,  
Yokohama, Midori-ku, 226-8501, Japan  
SOURCE: Tetrahedron Letters (2001), 42(15), 2817-2820  
CODEN: TELEAY; ISSN: 0040-4039  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 135:46021  
IT 344362-58-9P 344362-59-0P 344362-62-5P  
344362-63-6P 344614-27-3P 344614-32-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
RACT  
(Reactant or reagent)  
(total synthesis of macrosphelides C and F)  
RN 344362-58-9 CAPLUS  
CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12,15-tetrone,  
4,10,16-trimethyl-, (4S,7E,10S,13E,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

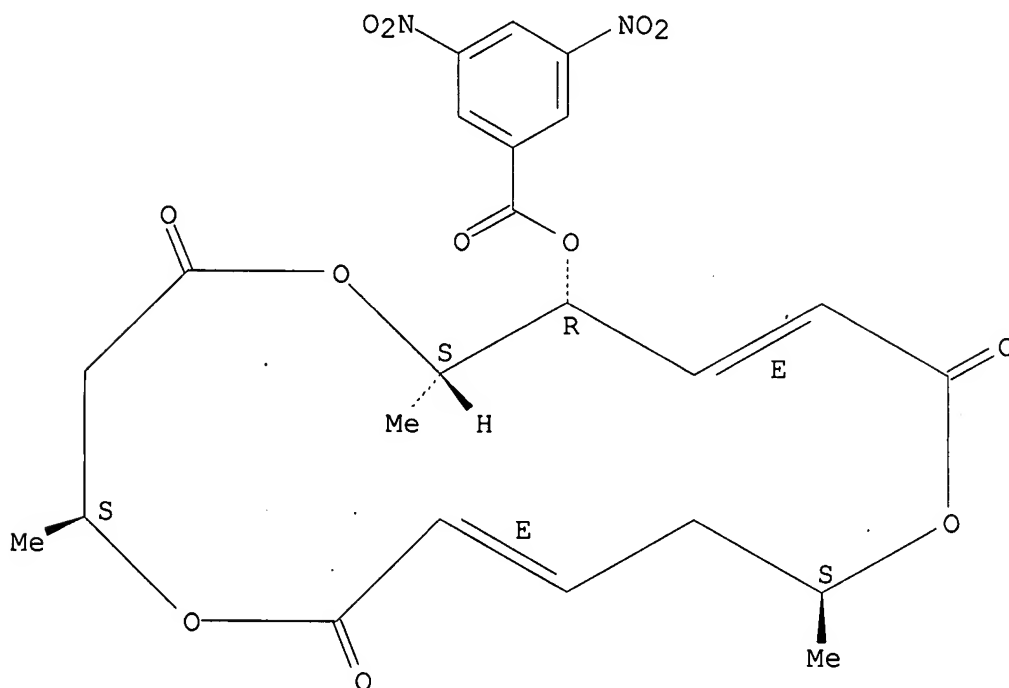


RN 344362-59-0 CAPLUS

10/535,136

CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12-trione, 15-[(3,5-dinitrobenzoyl)oxy]-4,10,16-trimethyl-, (4S,7E,10S,13E,15R,16S)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

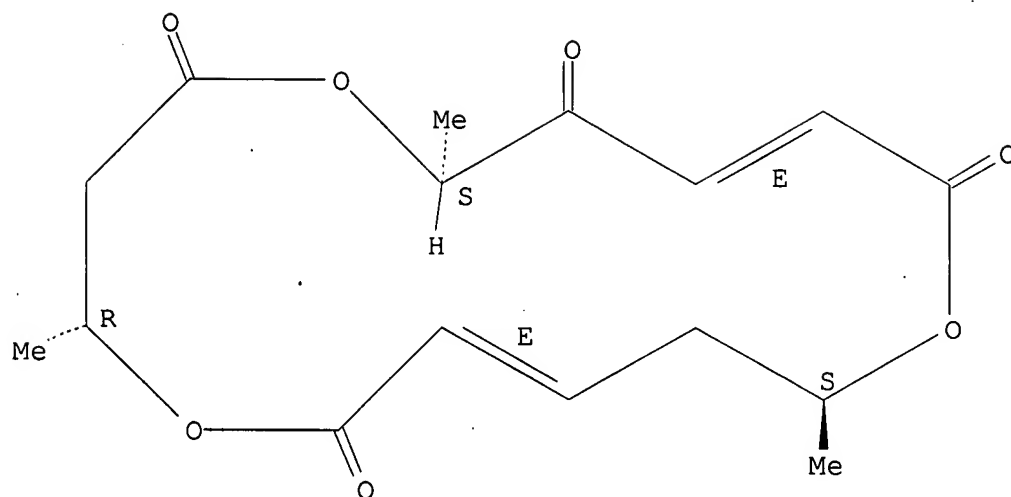


RN 344362-62-5 CAPLUS

CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12,15-tetrone,  
4,10,16-trimethyl-, (4R,7E,10S,13E,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

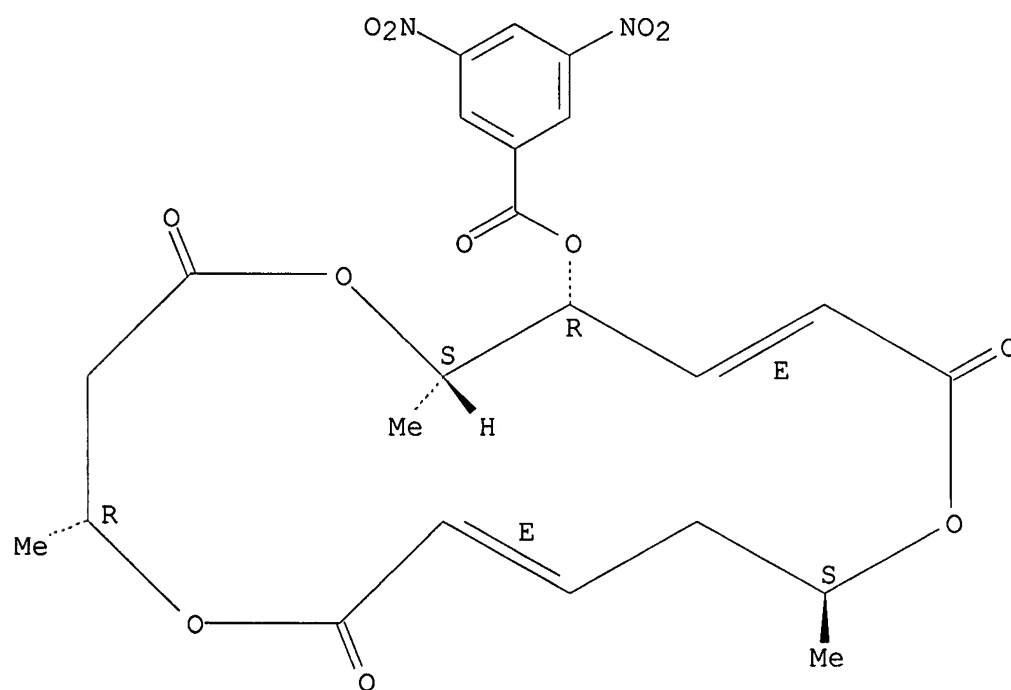
10/535,136



RN 344362-63-6 CAPLUS

CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12-trione, 15-[(3,5-dinitrobenzoyl)oxy]-4,10,16-trimethyl-, (4R,7E,10S,13E,15R,16S)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

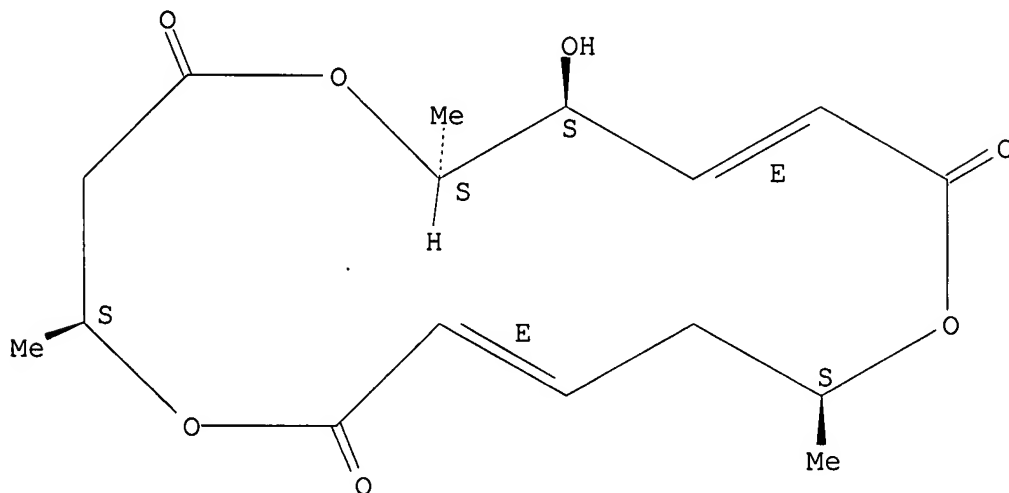


RN 344614-27-3 CAPLUS

10/535,136

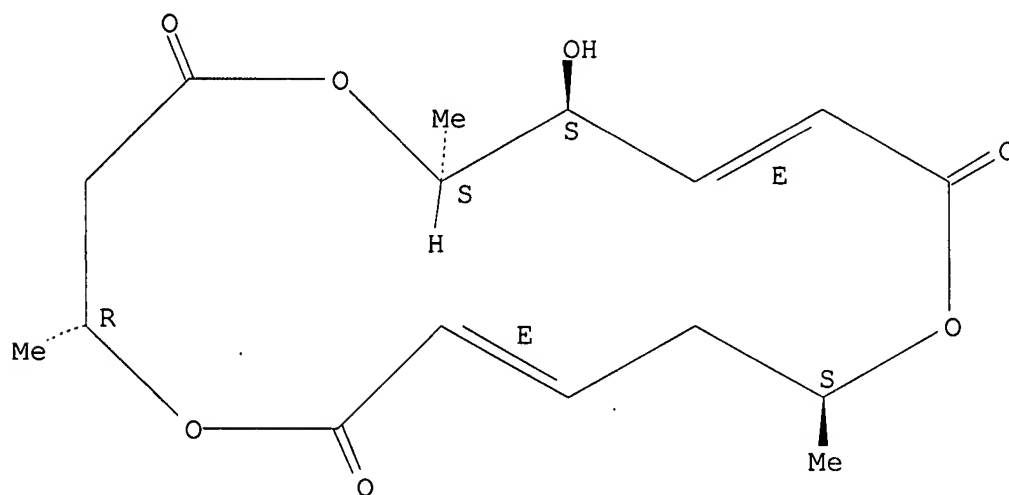
CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12-trione,  
15-hydroxy-4,10,16-  
trimethyl-, (4S,7E,10S,13E,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



RN 344614-32-0 CAPLUS  
CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12-trione,  
15-hydroxy-4,10,16-  
trimethyl-, (4R,7E,10S,13E,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



IT 199731-56-1P 200335-77-9P

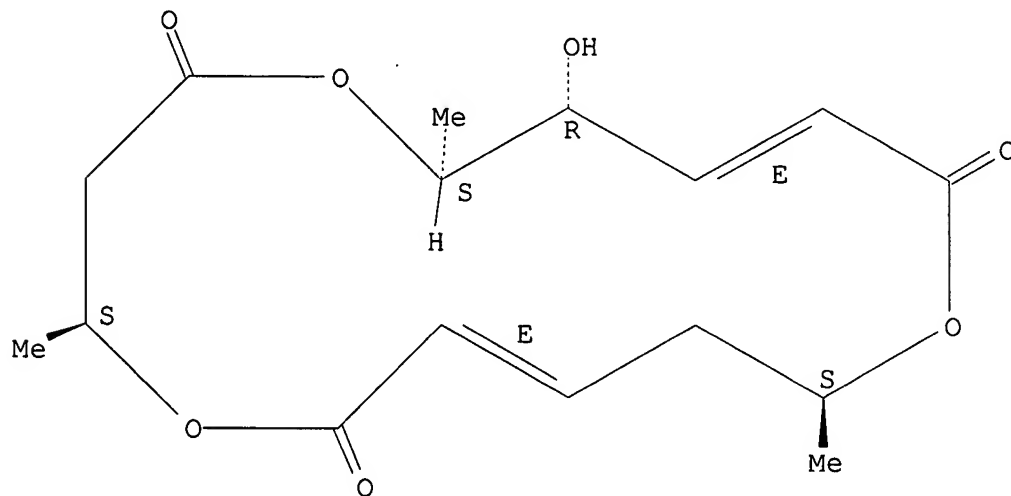
10/535,136

RL: SPN (Synthetic preparation); PREP (Preparation)  
(total synthesis of macrospinelides C and F)

RN 199731-56-1 CAPLUS

CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12-trione,  
15-hydroxy-4,10,16-  
trimethyl-, (4S,7E,10S,13E,15R,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).  
Double bond geometry as shown.

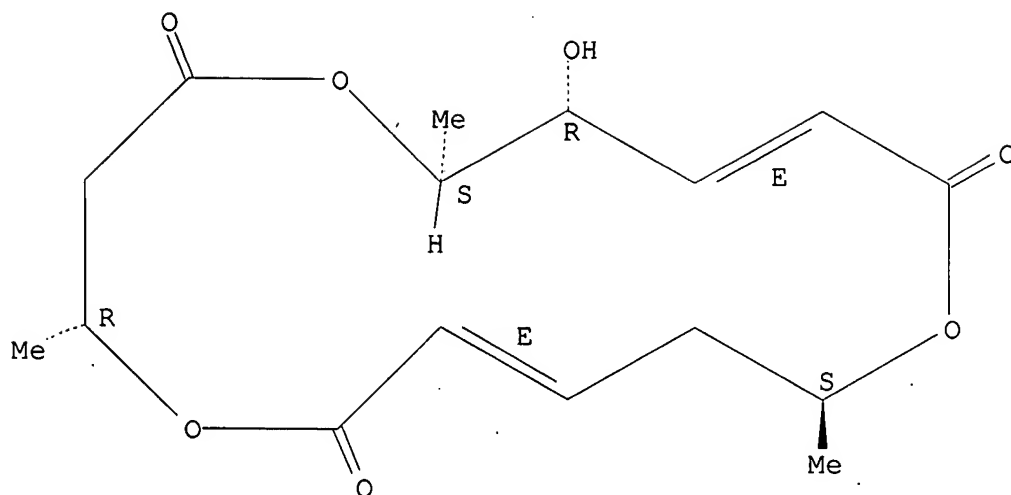


RN 200335-77-9 CAPLUS

CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12-trione,  
15-hydroxy-4,10,16-  
trimethyl-, (4R,7E,10S,13E,15R,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).  
Double bond geometry as shown.





AB Macrophelides C and F were synthesized by lactonization of 14-oxo seco acids at the O(10)-C(11) bond followed by reduction and Mitsunobu inversion of the resulting hydroxyl group. The seco acids were prepared from the corresponding furans by furan ring-opening with NBS followed by further oxidation of the 4-oxo-2-alkenals with NaClO<sub>2</sub>.  
 REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS

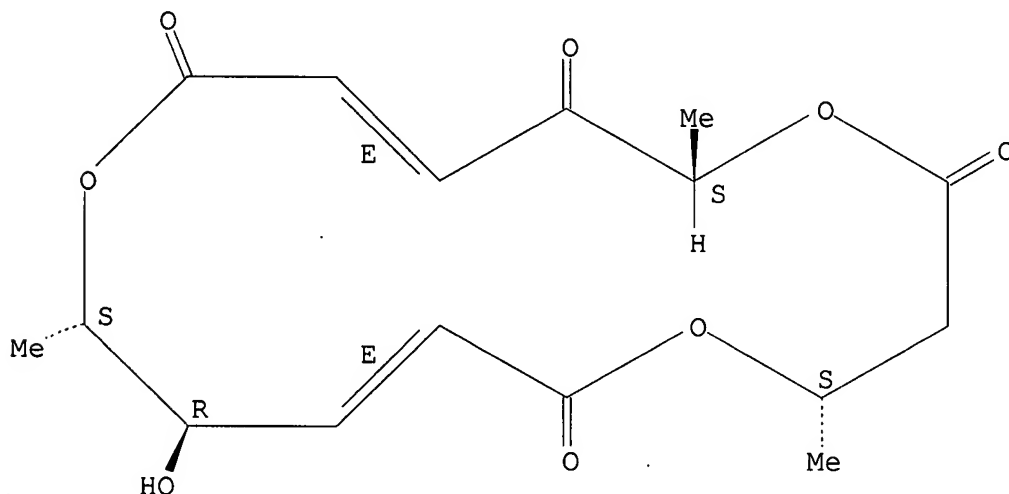
RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

L5 ANSWER 37 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1997:665088 CAPLUS  
 DOCUMENT NUMBER: 127:293063  
 TITLE: Relative and Absolute Stereochemistries and Total Synthesis of (+)-Macrophelides A and B, Potent, Orally Bioavailable Inhibitors of Cell-Cell Adhesion  
 AUTHOR(S): Sunazuka, Toshiaki; Hirose, Tomoyasu; Harigaya, Yoshihiro; Takamatsu, Satoshi; Hayashi, Masahiko; Komiyama, Kanki; Omura, Satoshi; Sprengeler, Paul A.;  
 Smith, Amos B., III  
 CORPORATE SOURCE: Research Center for Biological Function The  
 Kitasato Institute, School of Pharmaceutical Sciences  
 Kitasato University, Tokyo, 108, Japan  
 SOURCE: Journal of the American Chemical Society (1997), 119(42), 10247-10248  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society

10/535,136

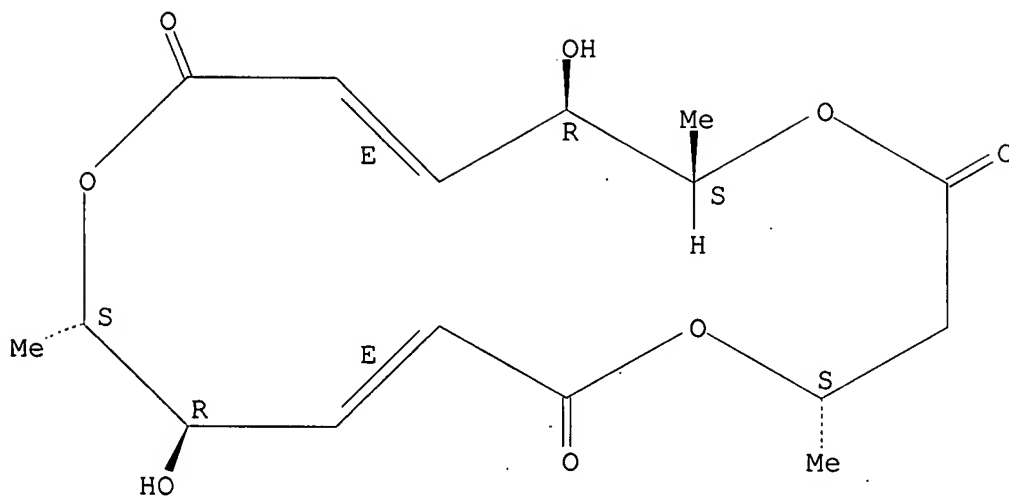
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 127:293063  
IT 172923-78-3P, Macrosphelide B  
RL: PNU (Preparation, unclassified); PREP (Preparation)  
(relative and absolute stereochemistries and total synthesis of  
(+)-macrosphelides a and B)  
RN 172923-78-3 CAPLUS  
CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12,15-tetrone,  
9-hydroxy-4,10,16-trimethyl-, (4S,7E,9R,10S,13E,16S)- (9CI) (CA INDEX  
NAME)

Absolute stereochemistry. Rotation (+).  
Double bond geometry as shown.



IT 172923-77-2P, Macrosphelide A  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(relative and absolute stereochemistries and total synthesis of  
(+)-macrosphelides a and B)  
RN 172923-77-2 CAPLUS  
CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12-trione, 9,15-dihydroxy-  
4,10,16-trimethyl-, (4S,7E,9R,10S,13E,15R,16S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).  
Double bond geometry as shown.



IT 196926-58-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

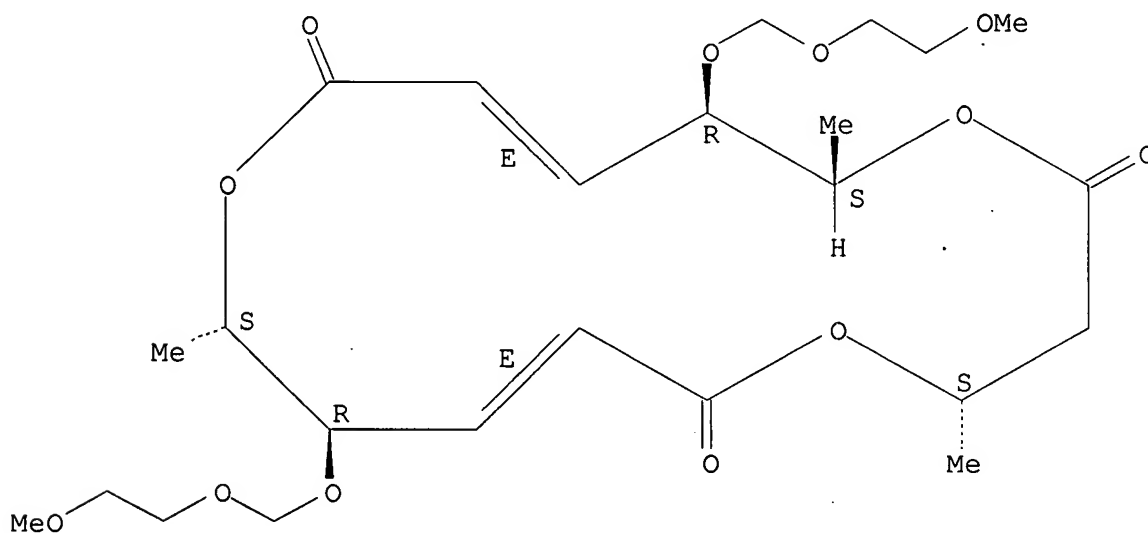
(relative and absolute stereochemistries and total synthesis of  
(+)-macrosphelides a and B)

RN 196926-58-6 CAPLUS

CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12-trione, 9,15-bis[(2-methoxyethoxy)methoxy]-4,10,16-trimethyl-, (4S,7E,9R,10S,13E,15R,16S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.



10/535,136

IT 196926-44-0P 196926-45-1P 196926-46-2P

196926-47-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(relative and absolute stereochemistries and total synthesis of  
(+)-macrosphelides a and B)

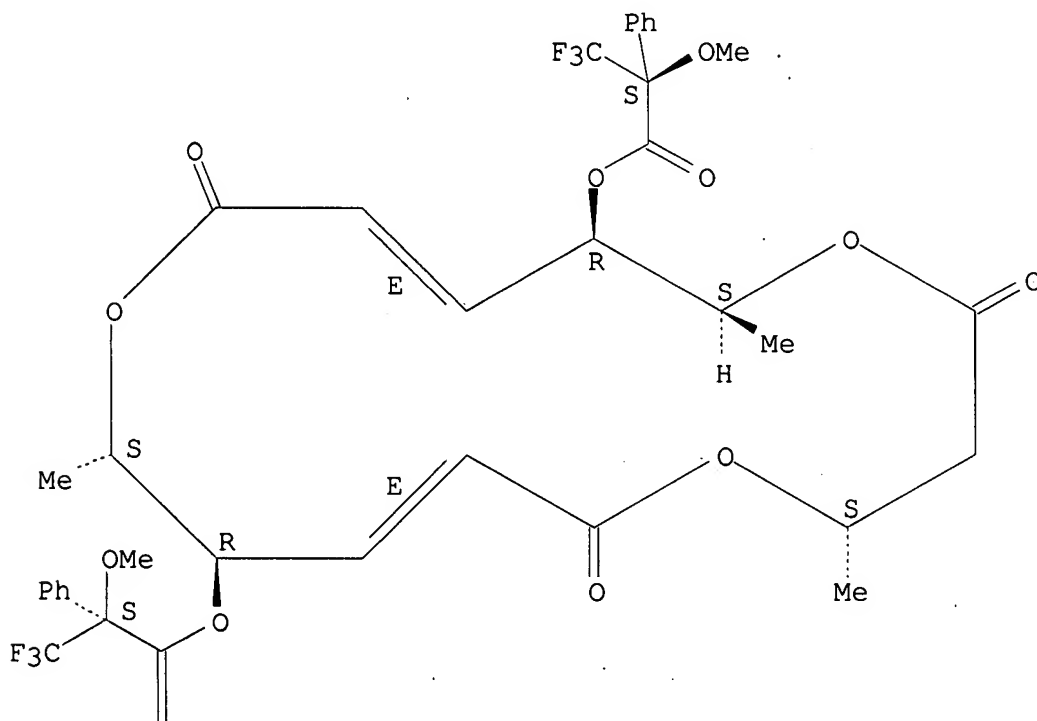
RN 196926-44-0 CAPLUS

CN Benzeneacetic acid,  $\alpha$ -methoxy- $\alpha$ -(trifluoromethyl)-,  
(2S,6S,7R,8E,12S,13R,14E)-2,6,12-trimethyl-4,10,16-trioxo-1,5,11-  
trioxacyclohexadeca-8,14-diene-7,13-diyl ester, ( $\alpha$ S, $\alpha'$ S)-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

PAGE 1-A



PAGE 2-A



RN 196926-45-1 CAPLUS

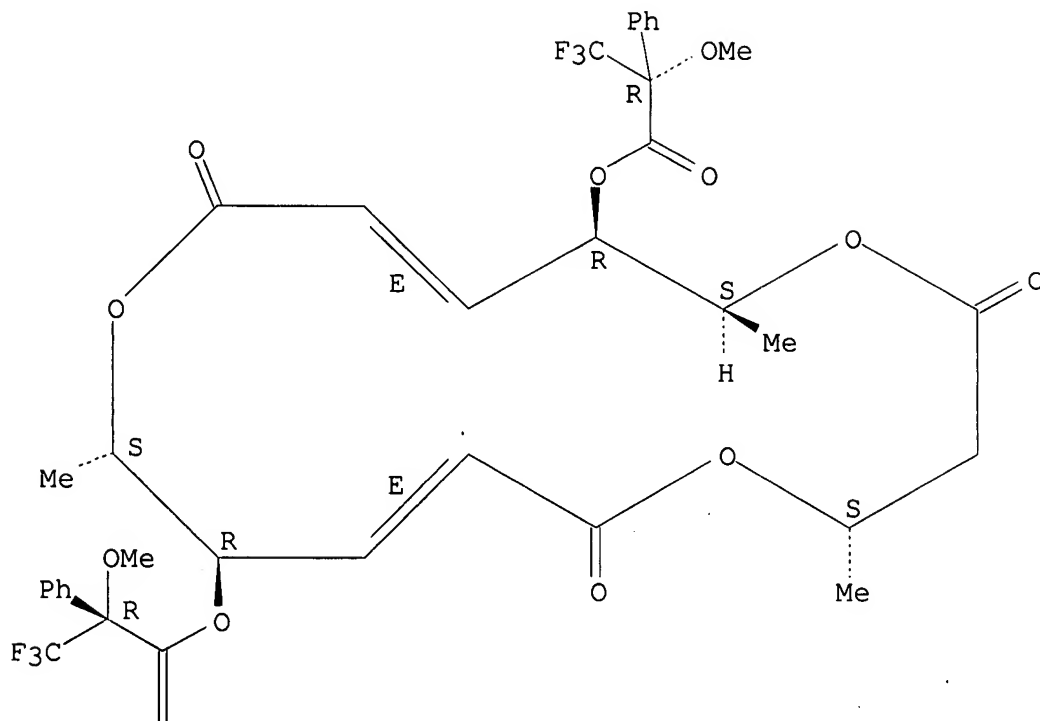
CN Benzeneacetic acid,  $\alpha$ -methoxy- $\alpha$ -(trifluoromethyl)-,  
(2S,6S,7R,8E,12S,13R,14E)-2,6,12-trimethyl-4,10,16-trioxo-1,5,11-  
trioxacyclohexadeca-8,14-diene-7,13-diyl ester, ( $\alpha$ R, $\alpha'$ R)-

10/535,136

(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).  
Double bond geometry as shown.

PAGE 1-A



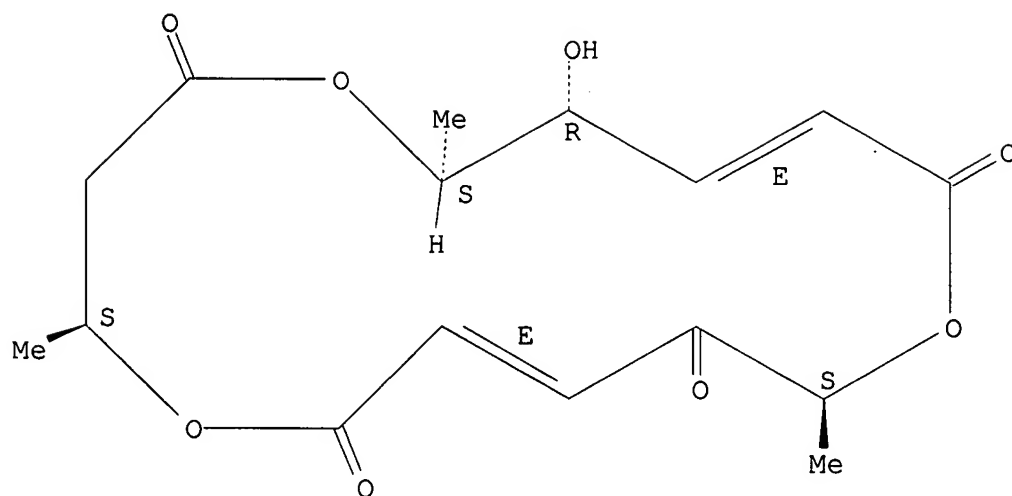
PAGE 2-A



RN 196926-46-2 CAPLUS  
CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,9,12-tetrone,  
15-hydroxy-4,10,16-trimethyl-, (4S,7E,10S,13E,15R,16S)- (9CI) (CA  
INDEX  
NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

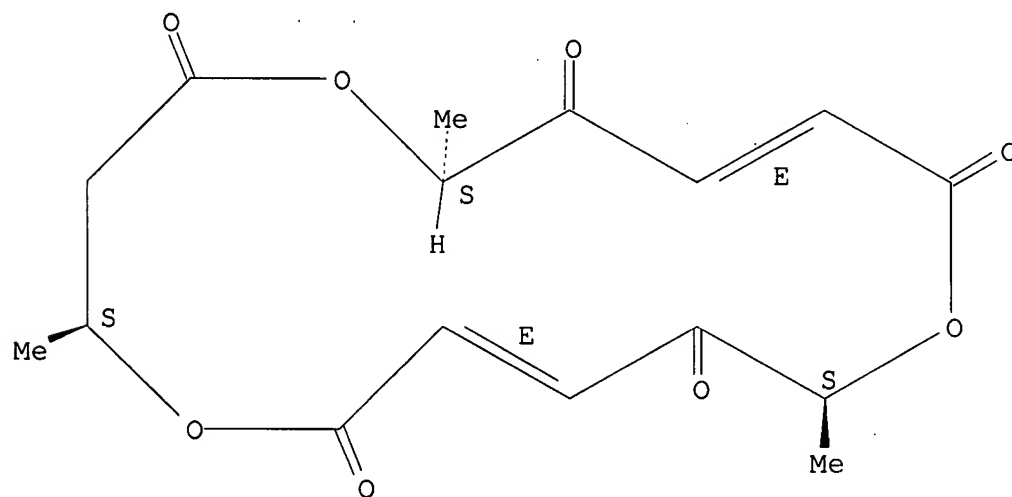
10/535,136



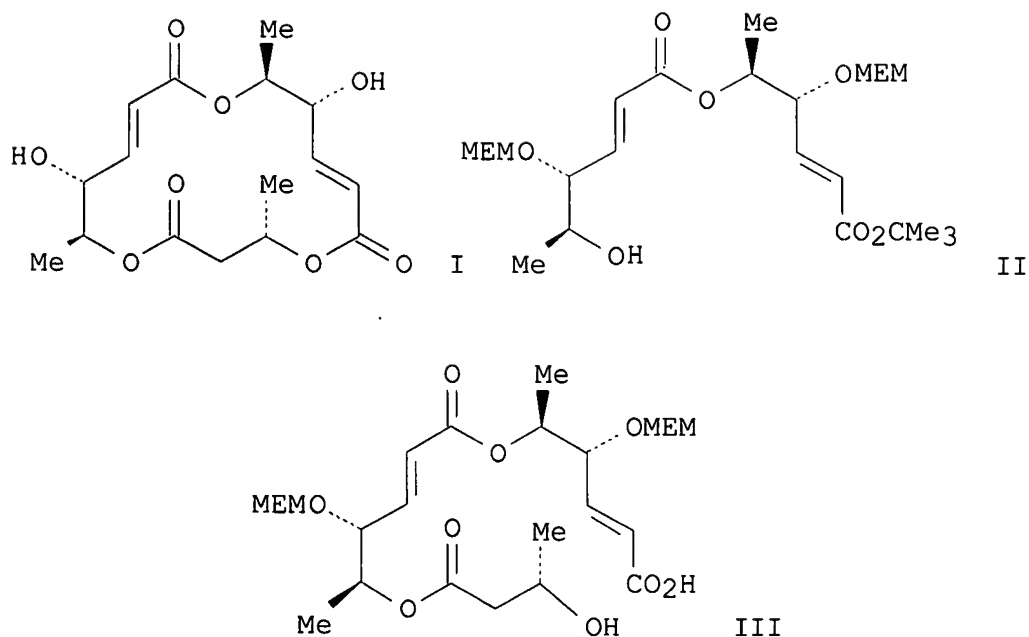
RN 196926-47-3 CAPLUS

CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,9,12,15-pentone,  
4,10,16-trimethyl-, (4S,7E,10S,13E,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



GI



AB (+)-Macrosphelides A (I) was prepared starting from E,E-MeCH:CHCH:CHCO<sub>2</sub>Me<sub>3</sub> via II and III. The successful route also constitutes a formal construction of (+)-Macrosphelide B, confirming the assigned structures of both congeners.

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS

FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

L5 ANSWER 38 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1996:76046 CAPLUS  
 DOCUMENT NUMBER: 124:175649  
 TITLE: Macrosphelide, a novel inhibitor of cell-cell adhesion

AUTHOR(S): molecule. II. Physicochemical properties and structural elucidation  
 Takamatsu, Satoshi; Kim, Yong-Pil; Hayashi, Masahiko;  
 Kanki; Hiraoka, Hidemi; Natori, Masahiko; Ko, iyama;

CORPORATE SOURCE: Omura, Satoshi  
 SOURCE: Kitasato Inst., Tokyo, 108, Japan  
 Journal of Antibiotics (1996), 49(1), 95-8  
 CODEN: JANTAJ; ISSN: 0021-8820  
 PUBLISHER: Japan Antibiotics Research Association  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

10/535,136

IT 172923-77-2, Macrosphelide A 172923-78-3, Macrosphelide B

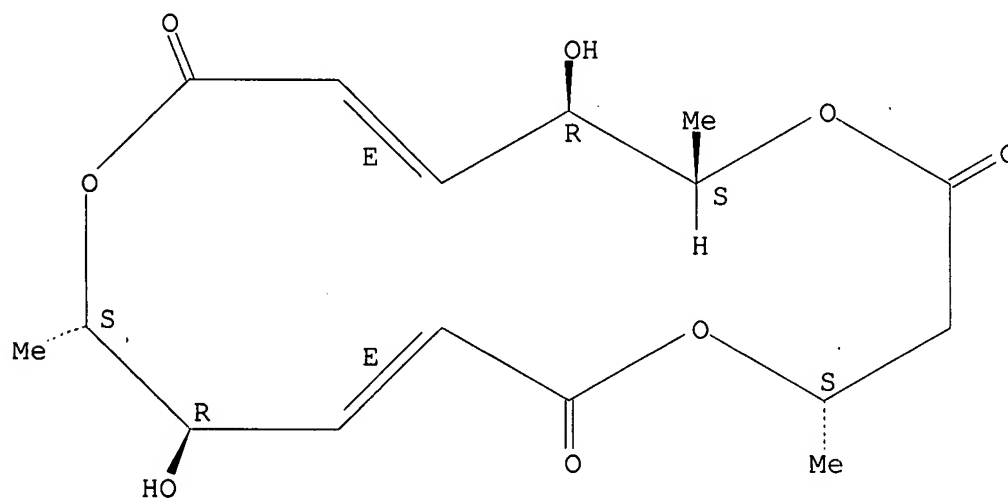
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
(physicochem. properties and structural elucidation of

macrosphelide)

RN 172923-77-2 CAPLUS

CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12-trione, 9,15-dihydroxy-4,10,16-trimethyl-, (4S,7E,9R,10S,13E,15R,16S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).  
Double bond geometry as shown.

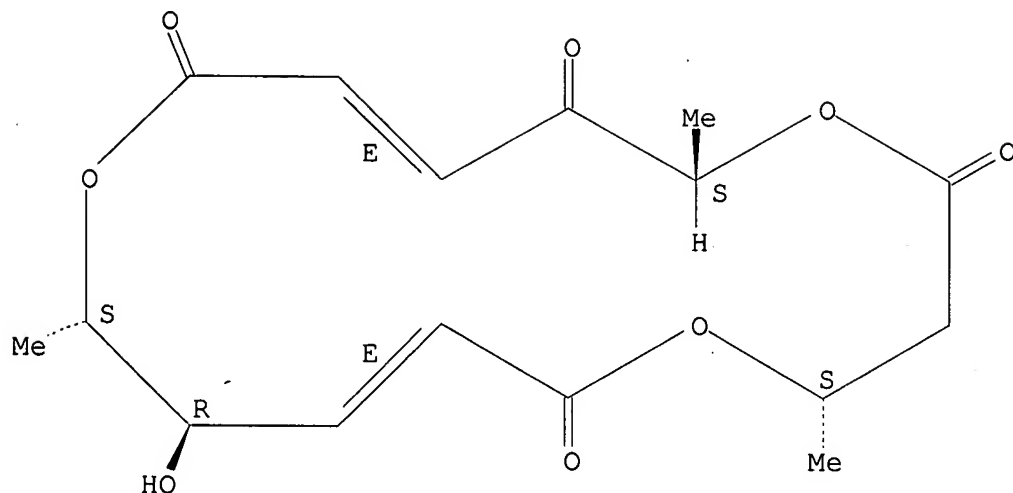


RN 172923-78-3 CAPLUS

CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12,15-tetrone, 9-hydroxy-4,10,16-trimethyl-, (4S,7E,9R,10S,13E,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).  
Double bond geometry as shown.





IT 173991-58-7P 173991-59-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

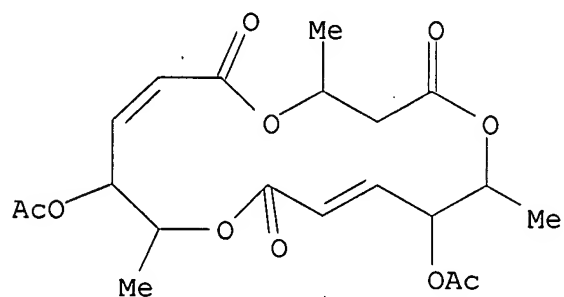
(physicochem. properties and structural elucidation of  
macrophelide)

RN 173991-58-7 CAPLUS

CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12-trione,  
9,15-bis(acetyloxy)-

4,10,16-trimethyl- (9CI) (CA INDEX NAME)

Currently available stereo shown.

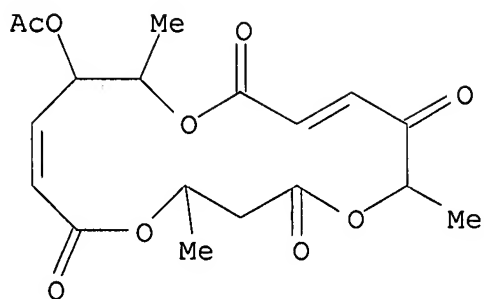


RN 173991-59-8 CAPLUS

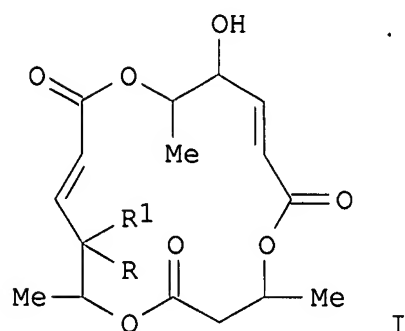
CN 1,5,11-Trioxacyclohexadeca-7,13-diene-2,6,12,15-tetrone,  
9-(acetyloxy)-4,10,16-trimethyl- (9CI) (CA INDEX NAME)

Currently available stereo shown.

10/535,136



GI



AB New anticell-adherence compds., macrosphelides A (I; R,R1 = H, OH) and B

(I; RR1 = O), were isolated from the fermentation broth of *Microsphaeropsis* sp.

FO-5050, and their structures were elucidated by spectroscopic methods and by chemical transformations. Macrosphelides A (M.W. 342, C16J22O8) and B (M.W. 340, C16H20O8) with three esters in their mols. were

classified as 16-membered macrocyclic compds. Macrosphelide B was found

to be a corresponding oxidative product of macrosphelide A at the C-14 position.

=> log y

COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE

ENTRY

219.63

SINCE FILE

ENTRY

-29.64

TOTAL

SESSION

391.94

TOTAL

SESSION

-29.64

10/535,136

STN INTERNATIONAL LOGOFF AT 14:15:06 ON 02 MAY 2007